

## Calculation of triple differential *K*-shell ionization cross sections of atoms

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**Abstract** In this communication, we report our calculations of triple differential *K*-shell ionization cross sections (differential in energy and angles of the scattered and ejected electrons) of atoms by relativistic electron impact using one photon exchange approximation. In the present investigation, we use Dirac plane waves for both incident and scattered electrons and Darwin and relativistic Sommerfeld-Maue wave functions to represent the bound and ejected electrons, respectively. It is demonstrated that the shift in the peak of the binary maxima and formation of the recoil peak in  $(e, 2e)$  collision occurs due to the interference between the atomic transition charge density and atomic transition current density contribution to the triple differential cross section (TDCS) in asymmetric geometry.

**Keywords** *K*-shell ionization, TDCS,  $(e, 2e)$  process

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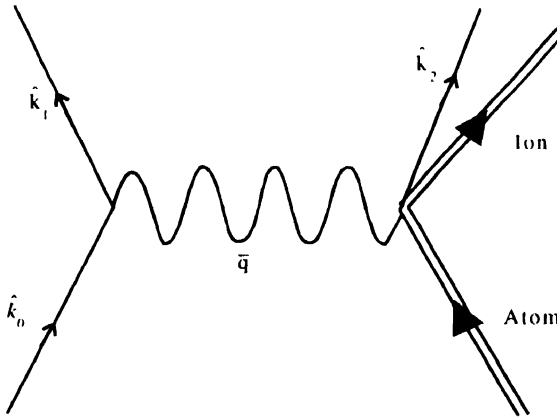
### 1. Introduction

The electron impact inner-shell ionization cross sections of atoms (differential in energy and angles of the ejected and scattered electrons) are sensitive to the details of the atomic wavefunctions as well as to the details of the influence of the atomic potential on the incoming and outgoing electrons and thus their study offers a sensitive test of theories. Since the first coincident measurement of  $(e, 2e)$  process on atoms by Ehrhardt *et al* [1] and Amaldi *et al* [2] extensive theoretical and experimental investigations have been done. We refer the reader, for details on  $(e, 2e)$  process for atoms, molecules and solids to the review work of Ehrhardt *et al* [3], Byron and Joachain [4] and McCarthy and Weigold [5, 6]. The absolute triple differential cross section (TDCS) for relativistic electron impact *K*-shell ionization of different targets ranging from copper ( $Z=29$ ) to uranium ( $Z=92$ ) have been measured by Nakel and collaborators [7-12]. Theoretical calculations of the differential cross section of *K*-shell ionization by electron impact have been performed by a number of workers [13-19]. Fuss *et al* [13] and Bell [14] have calculated triply differential *K*-shell ionization cross section of atoms in plane wave impulse approximation whereas Cavalli and Avaldi [15] have calculated in semi-classical impulse

approximation. The theoretical formalism of TDCS has been developed by Das and Konar [16] using the semi-relativistic Sommerfeld-Maue wave function for the slow electron whereas Jakubassa-Amundsen [17] used non-relativistic Coulomb wave function multiplied by a free Dirac spinor for both outgoing electrons while Walters *et al* [10] used semi-relativistic Coulomb wave function for the slow electron and plane wave for the fast electron. Jakubassa-Amundsen [17, 18] has calculated TDCS in Coulomb-Born approximation in which the continuum eigenstates of both electrons are described by Coulomb waves to an effective charge. Dreizler *et al* [19] have computed TDCS in relativistic distorted wave Born approximation in which incident and outgoing electrons are described in the field of atom or ion while the ionization is described in term of a first order electron-electron interaction. We present in Section 2, an outline of the theoretical formalism used by us to compute the triple differential *K*-shell ionization cross section. In Section 3, the results of the present calculation for copper and silver targets is presented.

## 2. Theory

We present in this section, the theoretical formalism in which we have used one photon exchange approximation to calculate triple differential *K*-shell ionization cross section of atoms. Feynman diagram of one photon exchange approximation for  $(e, 2e)$  inner shell ionization process is shown in Figure 1, where  $\hat{k}_0$  and  $\hat{k}_1$  represent the incident and scattered electron with four-momenta  $\hat{k}_0 \equiv (\frac{E_0}{c}, \mathbf{k}_0)$  and  $\hat{k}_1 \equiv (\frac{E_1}{c}, \mathbf{k}_1)$  in X-Z plane. The scattered electron makes an angle  $\theta_1$  with the incident electron beam axis. The electron emits a virtual photon carrying



**Figure 1.** Schematic diagram showing the four-momenta of the incident electron, scattered electron and ejected electron, respectively, indexed 0, 1 and 2  $\mathbf{q} = \mathbf{k}_0 - \mathbf{k}_1$  is the momentum transfer

momentum  $\mathbf{q}$  (in Z-direction) and energy  $\Delta E$  which impinges on the atom, resulting in knocking out of one inner shell electron (ejected electron) and an ion. The ejected electron has four-momenta  $\hat{k}_2 \equiv (\frac{E_2}{c}, \mathbf{k}_2)$  is moving in X-Z plane making an angle  $\theta_2$  with the electron beam axis. The  $\hat{q}_\mu \equiv (\frac{\Delta E}{c}, \mathbf{q})$  denotes the four-momenta transfer. The present formalism has been developed with the following assumptions [20] :

1. The incident and scattered electrons are described by Dirac plane waves.

2. A single inner shell bound electron in the process absorbs the virtual photon emitted by the incident electron.
3. The bound electron is described by Darwin wavefunction in Coulomb-potential

$$V(r) = -\frac{Z_{eff}}{|r|}.$$

4. The ejected electron is described by relativistic Sommerfeld-Maue wavefunction.

In electron scattering process, the main work is to evaluate the transition matrix element. We define the transition matrix element as :

$$M_\mu = -\frac{1}{c} \int J_\mu A^\mu d^3r, \quad (1)$$

where  $J_\mu$  is the atomic transition current given by  $J_\mu(r) = \bar{\phi}_{k,s} \hat{j}_\mu \phi_{1,\frac{1}{2},m_l}$  with  $\hat{j}_\mu$  representing the atomic transition current operator whereas  $\phi_{1,\frac{1}{2},m_l}$  and  $\phi_{k,s}$ , respectively the bound and ejected electron wavefunctions.  $A^\mu$  is the four potential generated by the electron current  $j_\mu$  and is simply given in terms of the retarded Green's function by

$$A_\mu(r) = \frac{1}{c} \int G(r_c, r) j_\mu(r_c) dr_c, \quad (2)$$

and

$$G(r_c, r) = \frac{e^{iM(r_c, r)}}{|r_c - r|}. \quad (3)$$

Here,  $j_\mu$  is the electron current and is given in terms of the incident and scattered electron wave functions :

$$J_\mu(r_c) = \bar{\psi}_s(r_c) \gamma_\mu \psi_i(r_c). \quad (4)$$

The triple differential cross section (TDCS) for the  $(e, 2e)$  process can be written as

$$\frac{d^3\sigma(e, 2e)}{dE_1 d\Omega_1 d\Omega_2} = \frac{2\pi}{4E_0 E_1} \cdot \frac{1}{I_m} \cdot \rho_{e_1} \cdot \rho_{e_2} \sum_{s, m_l} |\bar{M}_\mu|^2, \quad (5)$$

where  $I_m$  is the incoming electron flux ( $c^2 k_0 / E_0$ ), and  $\rho_{e_1}$  and  $\rho_{e_2}$  are the density of the final states have the same form for the outgoing scattered and ejected electrons and is given by the Fermi phase space is

$$\rho_{e_i} = \frac{k_i E_i}{(2\pi)^3 c^2}; \text{ with } i = 1, 2. \quad (6)$$

On squaring the matrix element (eq. 1), summing and averaging over electron spins, we obtain

$$|\bar{M}_\mu|^2 = \left[ \frac{4\pi}{q_\mu^2} \right]^2 \cdot [A_Q^2(s_2, m_k) + A_J^2(s_2, m_k) - 2A_{QJ}(s_2, m_k)] \quad (7)$$

and  $\sum_{s_2, m_k}$  is the sum to be taken over the spin states of the bound ( $m_k = \pm \frac{1}{2}$ ) and the ejected electron ( $s_2 = \pm \frac{1}{2}$ ).

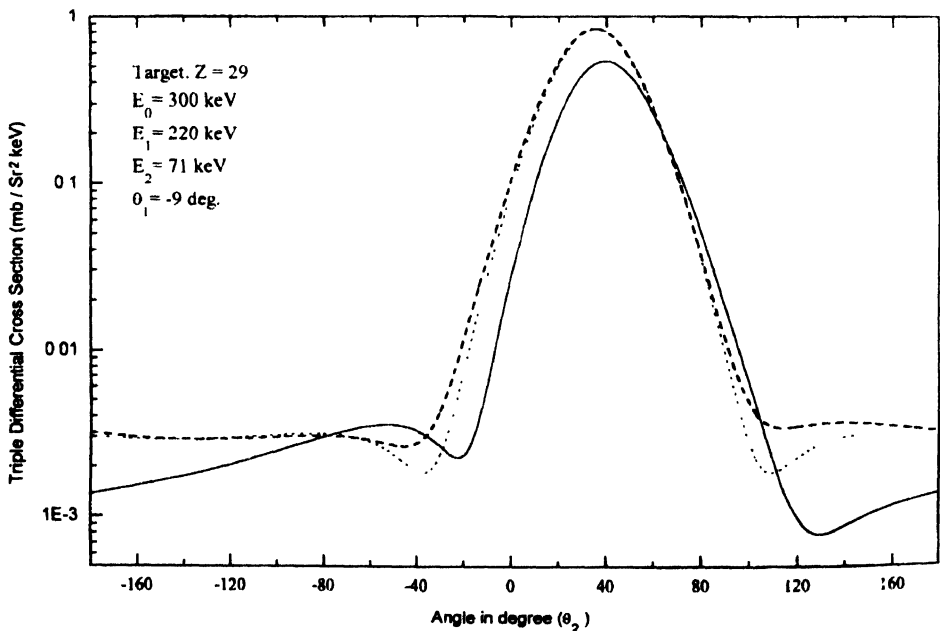
$A_Q^2(s_2, m_k)$ ,  $A_J^2(s_2, m_k)$  are the atomic transition charge density and atomic transition current density contribution and  $A_{QJ}(s_2, m_k)$  is an *interference term* between the atomic transition charge density and the atomic transition current density contributions. The expressions for these quantities are as follows :

$$A_Q^2(s_2, m_k) = \left( \frac{4E_0 E_1}{c^2} + q_\mu^2 \right) \cdot |Q_\mu(s_2, m_k)|^2, \quad (8)$$

$$A_J^2(s_2, m_k) = 4 \operatorname{Re} \left[ (k_0 \cdot J_\mu^*(s_2, m_k)) (k_1 \cdot J_\mu(s_2, m_k)) \right] - q_\mu^2 |J_\mu(s_2, m_k)|^2, \quad (9)$$

and 
$$A_{QJ}(s_2, m_k) = 2 \operatorname{Re} \left[ Q_\mu^*(s_2, m_k) \left( \frac{E_1}{c} k_0 + \frac{E_0}{c} k_1 \right) \cdot J_\mu(s_2, m_k) \right]. \quad (10)$$

Here  $Q_\mu(s_2, m_k)$  and  $J_\mu(s_2, m_k)$  are atomic transition charge density and atomic transition current density, respectively.



**Figure 2.** Triple different cross section ( $mb / sr^2$  keV) for *K*-shell ionization of copper ( $Z = 29$ ) plotted against scattering angle  $\theta_2$  (in degrees) of the ejected electrons ( $E_2 = 71$  keV) with incident electron energy  $E_0 = 300$  keV and scattered electron ( $E_1 = 220$  keV) being detected at  $\theta_1 = -9^\circ$ . The dashed and dotted curves represent, respectively the TDCS by including the contributions of the atomic transition charge density and atomic transition charge density plus atomic transition current density. The solid curve represents the TDCS by further including the interference term.

For brevity, the explicit expressions of  $A_Q^2(s_2, m_k)$ ,  $A_J^2(s_2, m_k)$  and  $A_{QJ}(s_2, m_k)$  are not presented here.

### 3. Results and discussion

In Figure 2, we have depicted the result of our calculation of K-shell ionization cross section of copper in coplanar asymmetric geometry at incident electron energy of  $E_0 = 300$  keV for two outgoing electrons having energies  $E_1 = 220$  keV and  $E_2 = 71$  keV at a scattering angle  $\theta_1 = -9^\circ$  (fast electron) as a function of detection angle  $\theta_2$  of the slow electron. In Figure 3 TDCS for silver target in coplanar asymmetric geometry is shown. Here the angle of the fast electron is fixed at  $-7^\circ$  and the energy values  $E_1 = 375$  keV and  $E_2 = 100$  keV for the incident electron impact energy  $E_0 = 500$  keV. In Figures 2 and 3 dashed curve represents the results of our calculation of TDCS by including the atomic transition charge density contribution only whereas the dotted curve depicts the contribution to the TDCS, due to atomic transition charge density as well as atomic transition current density. The solid curve in Figures 2 and 3 depicts the results of our calculation of TDCS by including the contributions of the atomic transition charge density, atomic transition current density as well as the *interference* between the atomic transition charge and current densities. The results presented in Figures 2 and 3 demonstrates that the shift in the peak of the binary maxima and the formation of recoil peak in  $(e, 2e)$  collision occurs due to the interference term to the TDCS in asymmetric geometry. We suggest here that there is a necessity of extensive computation on different incident electron energies at different targets to appreciate better the contribution to the binary and recoil peak due to the interference term. Extensive computation of the TDCS at relativistic incident electron energies and for different targets for available experimental data is in progress.

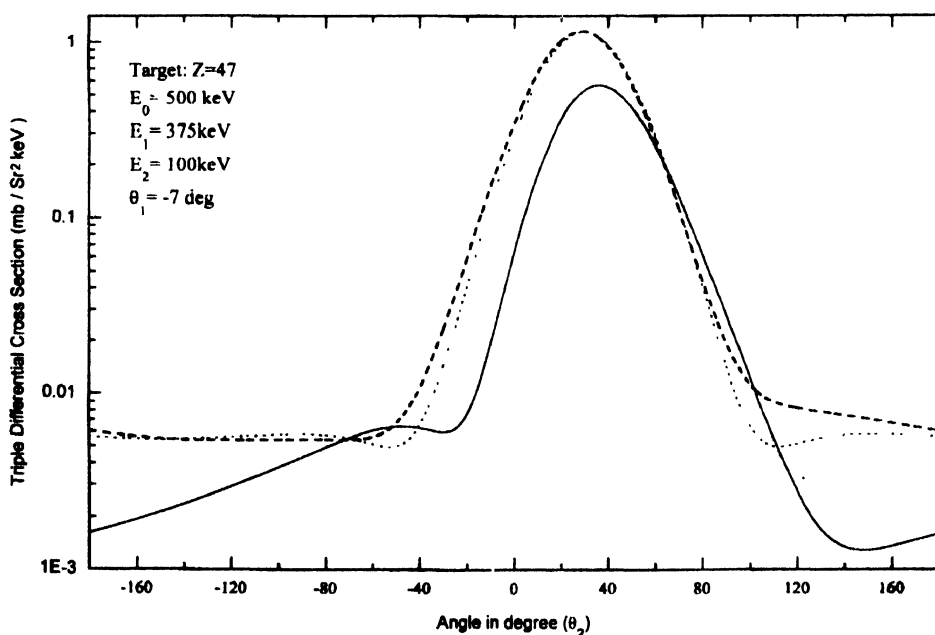


Figure 3. Same as in Figure 2 but for silver ( $Z = 47$ ) with  $E_0 = 500$  keV,  $E_2 = 100$  keV,  $E_1 = 375$  keV and  $\theta_1 = -7^\circ$ .

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